

Dimethylglyoxime

95-45-4 | DTXSID2044393

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 200 °C

Global applicability domain: Inside

Local applicability domain index: 6.63e-01

Confidence level: 3.14e-01

Nearest Neighbors from the Training Set

Image not found

Dimethylglyoxime

Measured: 246

Predicted: 200

Image not found

NSC21363

Measured: 173

Predicted: 131

Image not found

1H-Imidazole, 1-acetyl-

Measured: 102

Predicted: 115

Image not found

1,6-Diisocyanatohexane

Measured: -67.0

Predicted: -21.3